



Techniques of Water-Resources Investigations  
of the United States Geological Survey

Chapter A1

A MODULAR THREE-DIMENSIONAL  
FINITE-DIFFERENCE GROUND-WATER  
FLOW MODEL

By Michael G. McDonald and  
Arlen W. Harbaugh

This chapter supersedes U.S. Geological  
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Book 6

MODELING TECHNIQUES

**DEPARTMENT OF THE INTERIOR**  
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## PREFACE

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# A MODULAR THREE-DIMENSIONAL FINITE-DIFFERENCE GROUND-WATER FLOW MODEL

By Michael G. McDonald and Arlen W. Harbaugh

## ABSTRACT

This report presents a finite-difference model and its associated modular computer program. The model simulates flow in three dimensions. The report includes detailed explanations of physical and mathematical concepts on which the model is based and an explanation of how those concepts are incorporated in the modular structure of the computer program. The modular structure consists of a Main Program and a series of highly independent subroutines called "modules." The modules are grouped into "packages." Each package deals with a specific feature of the hydrologic system which is to be simulated, such as flow from rivers or flow into drains, or with a specific method of solving linear equations which describe the flow system, such as the Strongly Implicit Procedure or Slice-Successive Overrelaxation.

The division of the program into modules permits the user to examine specific hydrologic features of the model independently. This also facilitates development of additional capabilities because new packages can be added to the program without modifying the existing packages. The input and output systems of the computer program are also designed to permit maximum flexibility.

Ground-water flow within the aquifer is simulated using a block-centered finite-difference approach. Layers can be simulated as confined, unconfined, or a combination of confined and unconfined. Flow associated with external stresses, such as wells, areal recharge, evapotranspiration, drains, and streams, can also be simulated. The finite-difference equations can be solved using either the Strongly Implicit Procedure or Slice-Successive Overrelaxation.

The program is written in FORTRAN 77 and will run without modification on most computers that have a FORTRAN 77 compiler. For each program module, this report includes a narrative description, a flow chart, a list of variables, and a module listing.

## CHAPTER 1

### INTRODUCTION

#### Purpose

Since their inception, the two- and three-dimensional finite-difference models described by Trescott (1975), Trescott and Larson (1976), and Trescott, Pinder, and Larson (1976) have been used extensively by the U.S. Geological Survey and others for the computer simulation of ground-water flow. The basic concepts embodied in those models have been incorporated in the model presented here. The primary objectives in designing a new ground-water flow model were to produce a program that could be readily modified, was simple to use and maintain, could be executed on a variety of computers with minimal changes, and was relatively efficient with respect to computer memory and execution time.

The model program documented in this report uses a modular structure wherein similar program functions are grouped together, and specific computational and hydrologic options are constructed in such a manner that each option is independent of other options. Because of this structure, new options can be added without the necessity of changing existing subroutines. In addition, subroutines pertaining to options that are not being used can be deleted, thereby reducing the size of the program. The model may be used for either two- or three-dimensional applications. Input procedures have been generalized so that each type of model input data may be stored and read from separate external files. Variable formatting allows input data arrays to be read in any format without modification to the program. The type of output that is available has also been generalized so that the user may select various model output options to suit a particular

need. The program was originally written using FORTRAN 66 (McDonald and Harbaugh, 1984). It has subsequently been modified to use FORTRAN 77. This report documents the FORTRAN 77 version. The program is highly portable; it will run, without modification, on most computers. On some computers, minor modification may be necessary or desirable. A discussion about program portability is contained in Appendix A.

The major options that are presently available include procedures to simulate the effects of wells, recharge, rivers, drains, evapotranspiration, and "general-head boundaries". The solution algorithms available include two iteration techniques, the Strongly Implicit Procedure (SIP) and the Slice-Successive Overrelaxation method (SSOR).

#### Organization of This Report

The purpose of this report is to describe the mathematical concepts used in this program, the design of the program, and the input needed to use the program. The program has been divided into a main program and a series of highly independent subroutines called modules. The modules, in turn, have been grouped into "packages." A package is a group of modules that deals with a single aspect of the simulation. For example, the Well Package simulates the effect of wells, the River Package simulates the effect of rivers, and the SIP Package solves a system of equations using the Strongly Implicit Procedure. Many of the packages represent options which the user may or may not have occasion to use. Each of the packages is described in a separate chapter of this report. Two preliminary chapters

describe topics relating to the overall program; Chapter 2 derives the finite-difference equation that is used in the model and Chapter 3 describes the overall design of the program. Chapter 14 describes utility modules that are used by various packages to perform special tasks. Appendices A-E cover topics relating to the operation of the model.

Chapters 4 through 13 describe individual packages. The description of each package consists of (1) a section entitled "Conceptualization and Implementation," (2) input instructions for the package, and (3) documentation of the individual modules contained in the package. The Conceptualization and Implementation section describes the physical and mathematical concepts used to build the package. For example, in the chapter describing the River Package, an equation is derived which approximates flow through a riverbed, and a discussion is provided to show how that equation can be incorporated into the finite-difference equation. Chapters 12 and 13 describe the solution procedures currently available in the model.

The input instructions in Chapters 4 through 13 are presented in terms of input "items." An item of input may be a single record or a collection of similar records, or it may be an array or a collection of arrays. (In the model described herein, three-dimensional arrays are always read as a collection of two-dimensional arrays, one associated with each model layer.) The input section in each chapter presents a list of the input items associated with the package described in that chapter; the entries in this list are numbered, and generally consist of two lines (sometimes followed by a note or comment). For items which consist of a single record or a group of similar records, the first line in the entry gives the names of the fields comprising the records, while the second line shows the format of those fields, in standard FORTRAN notation. For an input item which consists of an array, the first

line of the entry gives the name of the array, while the second line gives the name of the utility module which reads the array. Further details concerning utility modules are provided in Chapter 14.

For most of the packages, the list of input items is subdivided into two major sections. One of these falls under the heading "FOR EACH SIMULATION" and includes all items for which only one entry is needed in each simulation; the other falls under the heading "FOR EACH STRESS PERIOD", and includes those items for which several entries may be needed in each simulation (for example, pumping rate, which may change with time during the period represented in a simulation). These major sections of the input list are further subdivided by headings which indicate the modules (subroutines) which read the item, or, in the case of an array, which call a utility subroutine to read the array. Input items that are printed entirely in capital letters are used as FORTRAN variables or arrays in the model program; input items which appear in mixed upper and lower case print are terms used in the instructions to describe the input fields or procedures, and do not appear in the model itself as FORTRAN variables. Chapter 4, which describes the Basic Package, includes two lists of input items; one of these describes input which is always required, while the other describes input associated with the optional "output control" section of the Basic Package.

An explanation of input fields is presented following the list of input items in Chapters 4 through 13. This explanation is followed in most cases by a sample input for the package under consideration. In Chapter 4, again, the input items associated with the output control option are treated separately; thus an independent explanation of fields and sample input are

provided for output control.

In each simulation, the user must designate which of the options of the program are to be utilized, and must indicate the file from which the input for each option is to be read. This is done through a one-dimensional array, IUNIT; the entries in this array are the unit numbers associated with the required files by the computer operating system. A location in the IUNIT array is given at the beginning of the input sections in Chapters 5 through 13, and at the beginning of the input discussion for "output control" in Chapter 4. If the option is to be utilized, the user must enter, in the designated IUNIT array location, the unit number of the file or channel through which input for the option is to be read; if the option is not required a zero is entered in this location. Further discussion of the IUNIT array is provided in Chapters 3 and 4.

Following the input section in Chapters 4 through 13, each chapter provides a documentation of the modules making up the associated package. This documentation consists of a list of the modules in the package, followed by detailed descriptions of each of the modules. The detailed description of a module generally contains four documents: (1) a narrative description of the module, (2) a flow chart of the module, (3) a FORTRAN listing of the module, and (4) a list of the variable names which are used in the module. For very simple modules, the flow chart is omitted. The narrative description is a numbered list of the functions performed by the module showing the order in which they are performed. The flow chart is a graphic equivalent of the narrative. The blocks in the flow chart are numbered with the same numbers used in the narrative so that the two documents can be cross referenced. An explanation of terms used in the flow chart is contained on the sheet

with the flow chart. The program listing contains comments with numbers corresponding to those used in the flow charts and the narratives. The fourth record of the listing contains a comment showing the time and day that the module was last modified. The list of variables shows the name, range, and definition of every variable used in the module. If the variable is used only in that module, its range is given as "Module"; if it is used in other modules of the package, but not outside the package, its range is given as "Package"; if it is used in the modules of more than one package, its range is given as "Global."

To summarize the organization of this report, Chapters 2 and 3, and the "Conceptualization and Implementation" section of Chapter 4, provide discussions relevant to the overall design and functioning of the program; the formulation of coefficients representing flow within the aquifer is discussed under "Conceptualization and Implementation" in Chapter 5; Chapters 6 through 11 provide discussions of particular external sources or sinks and their representation in the model; and Chapters 12 and 13 discuss the operation of particular solvers for the systems of finite difference equations generated in the model. Input instructions for each package are provided in the relevant chapter; a discussion of input for utility modules is provided in Chapter 14. The appendices provide a sample problem, abbreviated input instructions, and discussions of certain computer-related topics.

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## CHAPTER 2

### DERIVATION OF THE FINITE-DIFFERENCE EQUATION

#### Mathematical Model

The three-dimensional movement of ground water of constant density through porous earth material may be described by the partial-differential equation

$$\frac{\partial}{\partial x} \left( K_{xx} \frac{\partial h}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{yy} \frac{\partial h}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_{zz} \frac{\partial h}{\partial z} \right) - W = S_s \frac{\partial h}{\partial t} \quad (1)$$

where

$K_{xx}$ ,  $K_{yy}$  and  $K_{zz}$  are values of hydraulic conductivity along the  $x$ ,  $y$ , and  $z$  coordinate axes, which are assumed to be parallel to the major axes of hydraulic conductivity ( $Lt^{-1}$ );

$h$  is the potentiometric head ( $L$ );

$W$  is a volumetric flux per unit volume and represents sources and/or sinks of water ( $t^{-1}$ );

$S_s$  is the specific storage of the porous material ( $L^{-1}$ ); and

$t$  is time ( $t$ ).

For a derivation of equation (1) see for example Rushton and Redshaw (1979).

In general,  $S_s$ ,  $K_{xx}$ ,  $K_{yy}$ , and  $K_{zz}$  may be functions of space ( $S_s = S_s(x,y,z)$ ,  $K_{xx} = K_{xx}(x,y,z)$ , etc.) and  $W$  may be a function of space and time ( $W = W(x,y,z,t)$ ); equation (1) describes ground-water flow under nonequilibrium conditions in a heterogeneous and anisotropic medium, provided the principal axes of hydraulic conductivity are aligned with the coordinate directions.

Equation (1), together with specification of flow and/or head conditions at the boundaries of an aquifer system and specification of initial-head conditions, constitutes a mathematical representation of a ground-water flow system. A solution of equation (1), in an analytical sense, is an algebraic expression giving  $h(x,y,z,t)$  such that, when the derivatives of  $h$  with

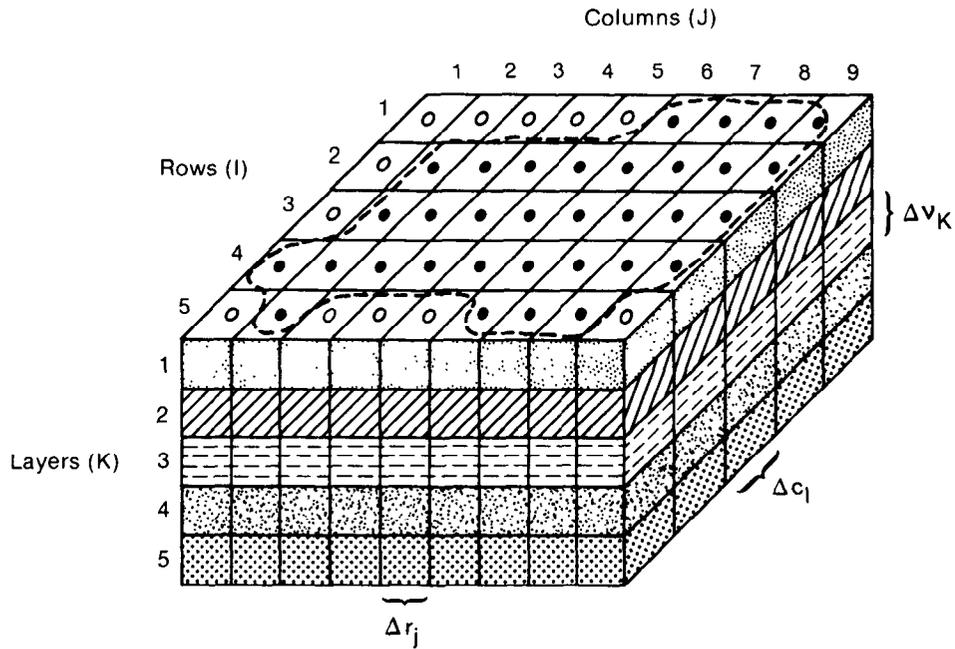
respect to space and time are substituted into equation (1), the equation and its initial and boundary conditions are satisfied. A time-varying head distribution of this nature characterizes the flow system, in that it measures both the energy of flow and the volume of water in storage, and can be used to calculate directions and rates of movement.

Except for very simple systems, analytical solutions of equation (1) are rarely possible, so various numerical methods must be employed to obtain approximate solutions. One such approach is the finite-difference method, wherein the continuous system described by equation (1) is replaced by a finite set of discrete points in space and time, and the partial derivatives are replaced by terms calculated from the differences in head values at these points. The process leads to systems of simultaneous linear algebraic difference equations; their solution yields values of head at specific points and times. These values constitute an approximation to the time-varying head distribution that would be given by an analytical solution of the partial-differential equation of flow.

The finite-difference analog of equation (1) may be derived by applying the rules of difference calculus; however, in the discussion presented here, an alternative approach is used with the aim of simplifying the mathematical treatment and explaining the computational procedure in terms of familiar physical concepts regarding the flow system.

#### Discretization Convention

Figure 1 shows a spatial discretization of an aquifer system with a mesh of blocks called cells, the locations of which are described in terms of rows, columns, and layers. An  $i,j,k$  indexing system is used. For a system



Explanation

----- Aquifer Boundary

● Active Cell

○ Inactive Cell

$\Delta r_j$  Dimension of Cell Along the Row Direction. Subscript (J) Indicates the Number of the Column

$\Delta c_l$  Dimension of Cell Along the Column Direction. Subscript (I) Indicates the Number of the Row

$\Delta v_K$  Dimension of the Cell Along the Vertical Direction. Subscript (K) Indicates the Number of the Layer

Figure 1.—A discretized hypothetical aquifer system.

consisting of "nrow" rows, "ncol" columns, and "nlay" layers,  $i$  is the row index,  $i = 1, 2, \dots, nrow$ ;  $j$  is the column index,  $j = 1, 2, \dots, ncol$ ; and  $k$  is the layer index,  $k = 1, 2, \dots, nlay$ . For example, figure 1 shows a system with  $nrow = 5$ ,  $ncol = 9$ , and  $nlay = 5$ . In formulating the equations of the model, an assumption was made that layers would generally correspond to horizontal geohydrologic units or intervals. Thus in terms of Cartesian coordinates, the  $k$  index denotes changes along the vertical,  $z$ ; because the convention followed in this model is to number layers from the top down, an increment in the  $k$  index corresponds to a decrease in elevation. Similarly rows would be considered parallel to the  $x$  axis, so that increments in the row index,  $i$ , would correspond to decreases in  $y$ ; and columns would be considered parallel to the  $y$  axis, so that increments in the column index,  $j$ , would correspond to increases in  $x$ . These conventions were followed in constructing figure 1; however, applications of the model requires only that rows and columns fall along consistent orthogonal directions within the layers, and does not require the designation of  $x$ ,  $y$ , or  $z$  coordinate axes.

Following the conventions used in figure 1, the width of cells in the row direction, at a given column,  $j$ , is designated  $\Delta r_j$ ; the width of cells in the column direction at a given row,  $i$ , is designated  $\Delta c_i$ ; and the thickness of cells in a given layer,  $k$ , is designated  $\Delta v_k$ . Thus a cell with coordinates  $(i, j, k) = (4, 8, 3)$  has a volume of  $\Delta r_8 \Delta c_4 \Delta v_3$ .

Within each cell there is a point called a "node" at which head is to be calculated. Figure 2 illustrates, in two dimensions, two conventions for defining the configuration of cells with respect to the location of nodes--the block-centered formulation and the point-centered formulation. Both systems start by dividing the aquifer with two sets of parallel lines which are orthogonal. In the block-centered formulation, the blocks formed by the sets of parallel lines are the cells; the nodes are at the center of the cells. In the point-centered formulation, the nodes are at the intersection points of the sets of parallel lines, and cells are drawn around the nodes with faces halfway between nodes. In either case, spacing of nodes should be chosen so that the hydraulic properties of the system are, in fact, generally uniform over the extent of a cell. The finite-difference equation developed in the following section holds for either formulation; however, only the block-centered formulation is presently used in the model.

In equation (1), the head,  $h$ , is a function of time as well as space so that, in the finite-difference formulation, discretization of the continuous time domain is also required.

#### Finite-Difference Equation

Development of the ground-water flow equation in finite-difference form follows from the application of the continuity equation: the sum of all flows into and out of the cell must be equal to the rate of change in storage within the cell. Under the assumption that the density of ground water is constant, the continuity equation expressing the balance of flow for a cell is

$$\sum Q_i = S S \frac{\Delta h}{\Delta V} \quad (2)$$